Pressure dependence of critical temperature in MgB_2 and two bands Eliashberg theory

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The variation of the superconducting critical temperature T_c as a function of the pressure p in the magnesium diboride MgB_2 has been studied in the framework of two-bands Eliashberg theory and traditional phonon coupling mechanism. I have solved the two-bands Eliashberg equations using first-principle calculations or simple assumptions for the variation, with the pressure, of the relevant physical quantities. I have found that the experimental T_c versus p curve can be fitted very well and information can be obtained on the dependence of the electron-phonon interaction matrix $< I^2 >$ by pressure. The pressure dependence of the superconductive gaps Δ_σ and Δ_π is also predicted.

PACS numbers: 74.62.Fj; 74.62.-c; 74.20.Fg; 74.70.Ad, 74.25.Kc

In the last few years, there is an noticeable increase of the study of superconductivity in many elements under pressure [1], such as sulphur (T_c = 17 K), oxygen (T_c = 0.5 K), carbon in nanotube (T_c = 15 K) and diamond forms (T_c = 4) K, a non-magnetic state of iron (T_c = 1 K), and the light elements lithium (T_c = 20 K) and boron (T_c = 11 K). The application of external pressure to superconductors can drive the compounds towards or away from lattice instabilities by varying the principal parameters determining the superconducting properties (the electronic density of states at the Fermi energy, the characteristic phonon frequency, and the electron-phonon coupling constant), and it can be used to tune the T_c and the superconducting properties. Almost all of the superconducting metallic materials, unlike the previous simple elements, show a decrease of T_c with pressure. This negative pressure coefficient was attributed to the volume dependence of the electronic density of states at the Fermi energy and of the effective interaction between the electrons mediated by the electron-phonon coupling. Measurements of the influence of pressure on the transition temperature and critical field yield information on the interaction causing the superconductivity. Indeed, the pressure would seem to be a variables whose effects might be capable of immediate theoretical interpretation. The binary alloy MgB_2, superconductor [2], at ambient pressure, at $T = 40$ K has, under pressure, a behaviour similar to metallic materials. The magnesium diboride has stimulated intense investigation, both from the theoretical and the experimental point of view. Now the electronic structure of MgB_2 is well understood and the Fermi surface consists of two three-dimensional sheets, from the π bonding and antibonding bands, and two nearly cylindrical sheets from the two-dimensional σ bands [3]. There is a large difference in the electron-phonon coupling on different Fermi surface sheets and this fact leads to a multiband description of superconductivity. Theory indicates that the strongest coupling is realized for the near-zone center in-plane optical phonon (E_{2g} symmetry) related to vibration of the B atoms [1]. The superconductivity in MgB_2 has been deeply studied in the past three years and so also the effect of pressure on the superconductive properties. The effect of pressure on the superconducting properties of MgB_2 has been studied by several groups. All groups observed a decrease of T_c with increasing pressure [4, 5] and I want show that this decrease can be very well explained in the framework of the two bands Eliashberg theory. In the following I will refer to the paper of A.F.Goncharov [5] because in there are present both measurement of the variation of critical temperature and of phonon mode by means of Raman measurement, with the pressure and so I mainly refer to these experimental data. In fact only in this work there are all input parameters necessary to my model.

Let us start from the generalization of the Eliashberg theory [7, 8] for systems with two bands [9], that has already been used with success to study the MgB_2 and related systems [10, 11, 12, 13, 14, 15]. To obtain the gaps and the critical temperature within the s-wave, two-band Eliashberg model one has to solve four coupled integral equations for the gaps $\Delta_i(i\omega_n)$ and the renormalization functions $Z_i(i\omega_n)$:

$$\omega_n Z_i(i\omega_n) = \omega_n + \pi T \sum_{m,j} \Lambda_{ij}(i\omega_n - i\omega_m) N_Z^j(i\omega_m) + + \sum_j \Gamma^{ij} N_Z^j(i\omega_n) \quad (1)$$

$$Z_i(i\omega_n)\Delta_i(i\omega_n) = \pi T \sum_{m,j} [\Lambda_{ij}(i\omega_n - i\omega_m) - \mu_{ij}^*(\omega_c)] \cdot \cdot\theta(|\omega_c| - \omega_m) N_\Delta^j(i\omega_m) + \sum_j \Gamma^{ij} N_\Delta^j(i\omega_n) \quad (2)$$

where i, j are band indices, θ is the Heaviside function, ω_c is a cutoff energy, Γ^{ij} is the non-magnetic impurity scattering rate in the Born approximation and:

$$\Lambda_{ij}(i\omega_n - i\omega_m) = \int_0^{+\infty} \frac{d\omega \alpha_{ij}^2 F(\omega)}{(\omega_n - \omega_m)^2 + \omega^2} \quad (3)$$

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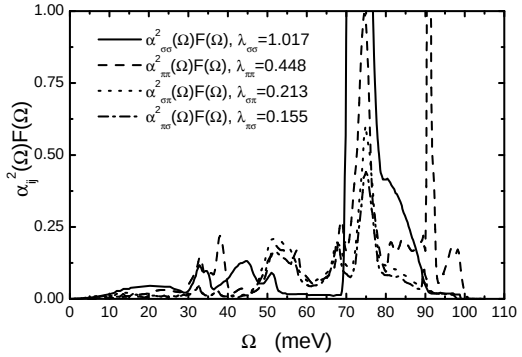

FIG. 1: The spectral functions of the two-band model for the MgB_2: $\sigma\sigma$ (solid line), $\pi\pi$ (dashed line), $\sigma\pi$ (dotted line) and $\pi\sigma$ (dashed dotted line), taken from ref. 11.

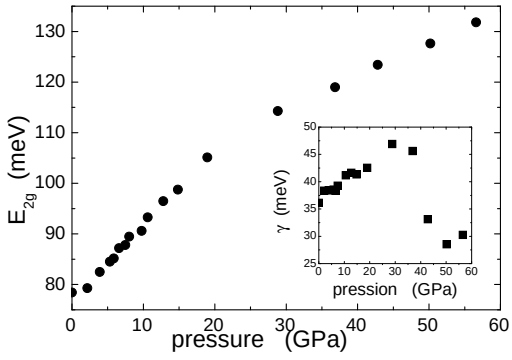

FIG. 2: Experimental energy of phonon E_{2g} of MgB_2 as a function of the pressure, see ref. 5. In the insert the experimental Raman linewidth as a function of the pressure, see always ref. 5.

$$N_{\Delta}^{j}(i\omega_m) = \frac{\Delta_j(i\omega_m)Z_j(i\omega_m)}{\sqrt{\omega_m^2 Z_j^2(i\omega_m) + \Delta_j^2(i\omega_m)Z_j^2(i\omega_m)}} \quad (4)$$

$$N_{Z}^{j}(i\omega_m) = \frac{\omega_m Z_j(i\omega_m)}{\sqrt{\omega_m^2 Z_j^2(i\omega_m) + \Delta_j^2(i\omega_m)Z_j^2(i\omega_m)}} \quad (5)$$

where $\omega_{\rm n} = \pi T(2n-1)$ and $n, m = 0, \pm1, \pm2....$

The solution of Eqs. 1,2 requires as input: i) the four (but only three independent[9]) electron-phonon spectral functions $\alpha_{ij}^2(\omega)F(\omega)$; ii) the four (but only three independent[9]) elements of the Coulomb pseudopotential matrix $\mu^*(\omega_{\rm c})$.

Let's start with the four spectral functions $\alpha_{ij}^2(\omega)F(\omega)$, that were calculated in ref. 11 (see Fig. 1).

For simplicity, I will assume that the shape of the $\alpha_{ij}^2F(\omega,p)$ functions does not change with the pressure, and I will only rescale them with the electron-phonon coupling constants λ_{ij}:

$$\alpha_{ij}^2F(\omega,p) = \frac{\lambda_{ij}(p)}{\lambda_{ij}(0)}\alpha_{ij}^2F(\omega,0) \quad (6)$$

Let me remind the definition of electron-phonon coupling constant [16, 17, 18]:

$$\lambda = \sum_{q,i}\frac{\gamma_i(q)}{\pi N_{\rm N}(E_{\rm F})\Omega_i^2(q)} \quad (7)$$

where $\gamma_i(q)$ is the phonon linewidth which is the width in energy of a phonon of momentum q, mode index i and energy $\Omega_i(q)$ and $N_{\rm N}(E_{\rm F})$ is the normal density of states at the Fermi level. The frequency Ω_i can be identified with the frequency of the B-B bond-stretching phonon mode (the $E_{2\rm g}$ mode), that has been recently measured as a function of pressure [5], and is reported in Fig. 2. In the insert of Fig. 2 the experimental Raman linewidth that here is used as phonon linewidth, is shown. Since this mode couples strongly with the holes on top of the

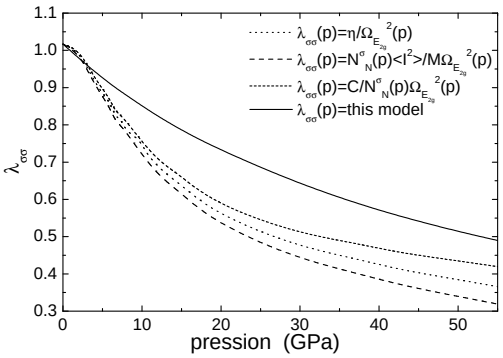

FIG. 3: Calculated electron-phonon coupling constant as a function of pressure in the four different cases: $\lambda_{\sigma\sigma}(p) = \eta/\Omega^2_{E_{2g}}(p)$ (dotted line), $\lambda_{\sigma\sigma}(p) = N^{\sigma}_{\rm N}(E_{\rm F},p) < I^2 > /2M\Omega^2_{E_{2g}}(p)$ (dashed line), $\lambda_{\sigma\sigma}(p) = C/(N^{\sigma}_{\rm N}(E_{\rm F},p)\Omega^2_{E_{2g}}(p))$ (short dashed line) and $\lambda_{\sigma\sigma}(p) = [\gamma(p)/\Omega^2_{E_{2g}}(p) + \pi\lambda_{\sigma\sigma}(0)N^{\sigma}_{\rm N}(E_{\rm F},0) - \gamma(0)/\Omega^2_{E_{2g}}(0)]/\pi N^{\sigma}_{\rm N}(E_{\rm F},p)$ (solid line).

σ band, from eq. 7 I will have for $\lambda_{\sigma\sigma}$ (which gives the most important contribution to superconductivity in our system):

$$\lambda_{\sigma\sigma}(p) = \frac{1}{\pi N^{\sigma}_{\rm N}(E_{\rm F},p)}[\frac{\gamma_{\rm E_{2g}}(p)}{\Omega_{\rm E_{2g}}(p)} + \sum_{q,i}\frac{\gamma_{\rm i}(q)}{\Omega_{\rm i}(q)}] \quad (8)$$

$$\lambda_{\sigma\sigma}(p) = \frac{1}{\pi N^{\sigma}_{\rm N}(E_{\rm F},p)}[\frac{\gamma_{\rm E_{2g}}(p)}{\Omega_{\rm E_{2g}}(p)} + C(0)] \quad (9)$$

where

$$C(0) = \pi\lambda_{\sigma\sigma}(0)N^{\sigma}_{\rm N}(E_{\rm F},0) - \frac{\gamma_{\rm E_{2g}}(0)}{\Omega_{\rm E_{2g}}(0)} \quad (10)$$

When the lattice parameters of MgB_2 are modified by chemical substitutions the normal density of states, at

the Fermi level, in the π-band changes relatively little [19] and so I assume that, in the first approximation,

$$N^{\pi}_{\rm N}(E_{\rm F},p) = N^{\pi}_{\rm N}(E_{\rm F},0) \qquad (11)$$

and

$$N^{\sigma}_{\rm N}(E_{\rm F},p) = N^{\sigma}_{\rm N}(E_{\rm F},0) + p\frac{\partial N^{\sigma}_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0} \qquad (12)$$

I use the values calculated in ref. 10: $N^{\sigma}_{\rm N}(E_{\rm F},0) = 0.30061\ (eV unitcell)^{-1}$ and $N^{\pi}_{\rm N}(E_{\rm F},0) = 0.40359\ (eV unitcell)^{-1}$ for the MgB_2. So $\frac{\partial N^{\sigma}_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0}$ is the only true free parameter of the model. In this way, I assume that the change in the frequency of the E_{2g} phonon affects the coupling constant, while I neglect its influence on the shape of the electron-phonon spectral function [14]. For the other coupling constants, I will instead assume for simplicity

$$\forall (i,j) \neq (\sigma,\sigma) \qquad \lambda_{\rm ij}(p) = \frac{N^{j}_{\rm N}(E_{\rm F},p)}{N^{j}_{\rm N}(E_{\rm F},0)}\lambda_{\rm ij}(0) \qquad (13)$$

with [10, 11] $\lambda_{\sigma\sigma}(0) = 1.017$, $\lambda_{\pi\pi}(0)$=0.448, $\lambda_{\sigma\pi}(0)$=0.213 and $\lambda_{\pi\sigma}(0)$=0.155. At the end, in this approximate model of electron-phonon coupling constants only $\lambda_{\sigma\sigma}$ and $\lambda_{\pi\sigma}$ change with the pressure. This fact is in agreement with the results of ref. 20 where the authors find that $\lambda_{\pi\pi}$ is almost constant. Fig. 3 shows the calculated electron-phonon coupling constant $\lambda_{\sigma\sigma}$ as a function of the pressure.

As far as the Coulomb pseudopotential is concerned, let us start from its expression in pure MgB_2 [10, 11, 21]:

$$\mu^*(p) = \left| \begin{array}{cc} \mu^*_{\sigma\sigma} & \mu^*_{\sigma\pi} \\ \mu^*_{\pi\sigma} & \mu^*_{\pi\pi} \end{array} \right| =$$

$$= \mu(\omega_c) N^{tot}_{\rm N}(E_{\rm F},p) \left| \begin{array}{cc} \frac{2.23}{N^{\sigma}_{\rm N}(E_{\rm F},p)} & \frac{1}{N^{\sigma}_{\rm N}(E_{\rm F},p)} \\ \frac{1}{N^{\pi}_{\rm N}(E_{\rm F},p)} & \frac{2.48}{N^{\pi}_{\rm N}(E_{\rm F},p)} \end{array} \right| \qquad (14)$$

where $\mu(\omega_c)$ is a free parameter and $N^{tot}_{\rm N}(E_{\rm F},p)$ is the total normal density of states at the Fermi level. The numbers 2.23 and 2.48 in the Coulomb matrix have been calculated for the MgB_2 in ambient pressure but, as a first approximation, I will suppose them not to depend on the pressure. In this way, the elements of the Coulomb pseudopotential matrix, $\mu^*_{\rm ij}$, depend on the pressure only through the densities of states at the Fermi level. Now I can fix the cut-off energy (e.g., ω_c = 700 meV) so as to reduce the number of adjustable parameters to two: the prefactor in the Coulomb pseudopotential, $\mu(\omega_c)$ and $\frac{\partial N^{\sigma}_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0}$. For having T_c = 40.2 K I fix $\mu(\omega_c)$ equal to 0.00315 so there is only more a free parameter for fitting the experimental critical temperature as a function of pressure. Before of examining the fit of experimental data with the my $\lambda_{\sigma\sigma}$ model I can check the other possible choices for the electron-phonon coupling constants.

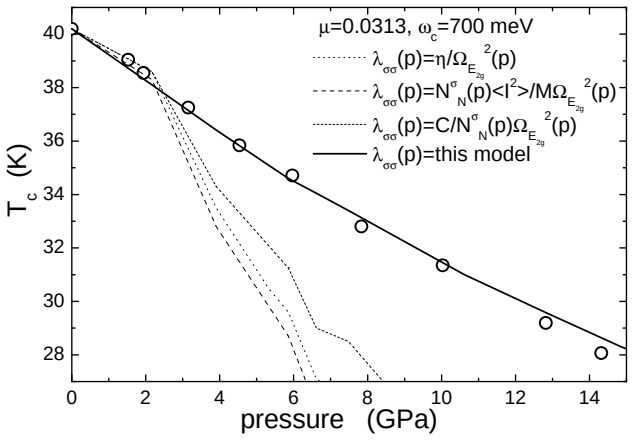

FIG. 4: The measured critical temperature T_c as function of the pressure (open circles) and theoretical fits obtained by different assumptions on the electron-phonon coupling constant $\lambda_{\sigma\sigma}(p) = \eta/\Omega^2_{E_{2g}}(p)$ (dotted line), $\lambda_{\sigma\sigma}(p) = N^{\sigma}_{\rm N}(E_{\rm F},p) < I^2 > /2M\Omega^2_{E_{2g}}(p)$ (dashed line), $\lambda_{\sigma\sigma}(p) = C/(N^{\sigma}_{\rm N}(E_{\rm F},p)\Omega^2_{E_{2g}}(p))$ (short dashed line) and $\lambda_{\sigma\sigma}(p) = [\gamma(p)/\Omega^2_{E_{2g}}(p) + \pi\lambda_{\sigma\sigma}(0)N^{\sigma}_{\rm N}(E_{\rm F},0) - \gamma(0)/\Omega^2_{E_{2g}}(0)]/\pi N^{\sigma}_{\rm N}(E_{\rm F},p)$ (solid line).

All cases are shown in Fig. 3. The first and simpler possibility is similar to the case of several transition metals [25]

$$\lambda(p) = \frac{\eta}{\Omega^2_{E_{2g}}(p)} \qquad (15)$$

where η is a constant [18, 23] and so

$$\lambda_{\sigma\sigma}(p) = \frac{\Omega^2_{E_{2g}}(0)}{\Omega^2_{E_{2g}}(p)}\lambda_{\sigma\sigma}(0) \qquad (16)$$

The result is in very poor agreement with experimental data (see dotted line in Fig. 4).

The second possibility is of that the effect of the pressure is similar to chemical substitutions as Al and C and so I assume that [14]

$$\lambda(p) = \frac{N_{\rm N}(E_{\rm F},p) < I^2 >}{M\Omega^2_{E_{2g}}(p)} \qquad (17)$$

where M is the ion mass [18] and $< I^2 >$ does not depend from the pressure. Consequently

$$\lambda_{\sigma\sigma}(p) = \frac{N^{\sigma}_{\rm N}(E_{\rm F},p)\Omega^2_{E_{2g}}(0)}{N^{\sigma}_{\rm N}(E_{\rm F},0)\Omega^2_{E_{2g}}(p)} \qquad (18)$$

$\frac{\partial N^{\sigma}_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0} = -0.003\ (eVGPa)^{-1}$. Also in this case the result is in very poor agreement with experimental data (see dashed line in Fig. 4).

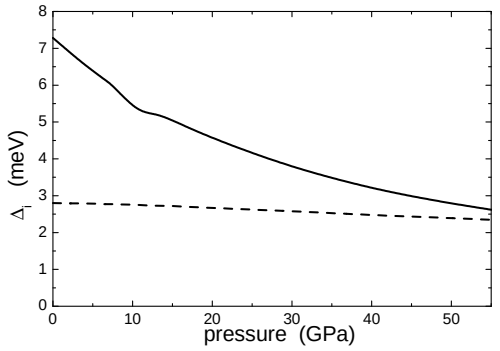

FIG. 5: The calculated values of the gap, at $T = 4.2$ K, Δ_σ (solid line) and Δ_π (dashed line) as a function of the pressure.

The last possibility is suggested by recent band-structure calculations that show MgB_2 is a traditional *sp* metal superconductor [3]. The pressure dependence of I has long been an interesting issue in the research of pressure effects in simple *sp* metals [26]. Zimans calculation of the electron-phonon interaction led to $< I^2 > \propto N_{\rm N}(E_{\rm F})^{-2}$, at least in the limit of long wavelengths [27]. So I find

$$\lambda_{\sigma\sigma}(p) = \frac{N^\sigma_{\rm N}(E_{\rm F},0)\Omega^2_{E_{2g}}(0)}{N^\sigma_{\rm N}(E_{\rm F},p)\Omega^2_{E_{2g}}(p)} \qquad (19)$$

and $\frac{\partial N^\sigma_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0} = -0.0007\ (eVGPa)^{-1}$. As in the previous cases the result is in very poor agreement with experimental data (see short dashed line in Fig. 4). Now I can see that my simple model is the alone that explains the experimental critical temperatures because other possible models for electron-phonon coupling constant $\lambda_{\sigma\sigma}$ are incompatible with experimental data. I obtain the best fit of experimental data (solid line in Fig. 4) with $\frac{\partial N^\sigma_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0} = 0.00584\ (eVGPa)^{-1}$. The fact that $N^\sigma_{\rm N}(E_{\rm F})$ increases with the pressure is in agreement with theoretical calculations [22]. The only free parameter of this model is $\frac{\partial N^\sigma_{\rm N}(E_{\rm F},p)}{\partial p}|_{p=0}$ and so when I have fixed the optimal value from the T_c fit I can calculate, in principle, all other physical quantities. In Fig. 5 the theoretical dependence of the σ and π gaps from the pressure is shown.

Now from the following equality

$$\frac{N^\sigma_{\rm N}(E_{\rm F},p) < I^2(p) >}{M\Omega^2_{\rm E_{2g}}(p)} = \frac{1}{\pi N^\sigma_{\rm N}(E_{\rm F},p)}[\frac{\gamma_{\rm E_{2g}}(p)}{\Omega_{\rm E_{2g}}(p)} + \sum_{q,i}\frac{\gamma_{\rm i}(q)}{\Omega_{\rm i}(q)}] \qquad (20)$$

it is possible determine the dependence of $N^\sigma_{\rm N}(E_{\rm F}) < I^2 >$ and of $< I^2 >$ from the pressure as it is shown in Fig 6. It can see that, after $\simeq 25$ GPa the Hopfield parameter [27] $N^\sigma_{\rm N}(E_{\rm F}) < I^2 >$ is almost constant.

At the end it is possible to use this model for explaining the experimental upper critical field [20] in function

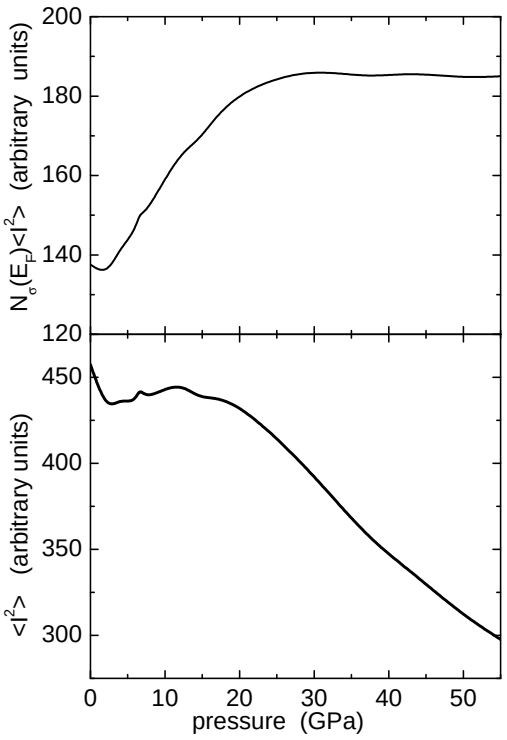

FIG. 6: Upper panel: the calculated value of $N^\sigma_{\rm N}(E_{\rm F}) < I^2 >$ of the σ-band as a function of pressure; lower panel: the calculated value of $< I^2 >$ of the σ-band as a function of pressure.

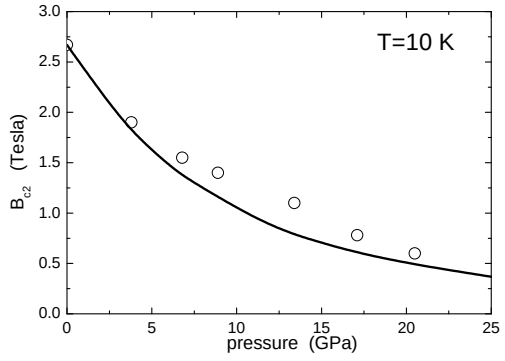

FIG. 7: The measured upper critical field (open circles), at T=10 K, from ref. 20, and the theoretical (solid line).

of pressure without free parameters. For the sake of completeness, I give here the linearized gap equations under magnetic field, for a superconductor in the clean limit (negligible impurity scattering), as can be found in ref. 20. In the following, v_{Fj} is the Fermi velocity of band j, and H_{c2} is the upper critical field:

$$\omega_n Z_i(i\omega_n) \ = \ \omega_n + \pi T \sum_{m,j} \Lambda_{ij}(i\omega_n - i\omega_m) sign(\omega_m) \qquad (21)$$

$$Z_i(i\omega_n)\Delta_i(i\omega_n) = \pi T\sum_{m,j}[\Lambda_{ij}(i\omega_n - i\omega_m) - \mu^*_{ij}(\omega_c)]\cdot \cdot\theta(|\omega_c| - \omega_m)\chi_j(i\omega_m)Z_j(i\omega_m)\Delta_j(i\omega_m) \quad (22)$$

$$\chi_j(i\omega_m) = (2/\sqrt{\beta_j})\int_0^{+\infty} dq\exp(-q^2)\cdot \cdot tan^{-1}[\frac{q\sqrt{\beta_j}}{|\omega_m Z_j(i\omega_m)| + i\mu_B H_{c2} sign(\omega_m)}] \quad (23)$$

with $\beta_j = \pi H_{c2} v^2_{Fj}/(2\Phi_0)$. In these equations the bare Fermi velocities are the input parameters $v_{Fj} = v^*_{Fj}\cdot\sum_i(1+\lambda_{ji})$ and are functions of p. For don't having free parameters I assume that, as in the free electron gas, $v_{Fj} \propto N^j_{\rm N}(E_{\rm F})$ and so $v_{Fj}(p) = v_{Fj}(0)N^j_{\rm N}(E_{\rm F},p)/N^j_{\rm N}(E_{\rm F},0)$. For obtaining exactly the upper critical field of MgB_2, in ambient pressure, I find $v^*_{F\sigma}(0) = 3.6\cdot 10^5$ m/s and $v^*_{F\pi}(0) = 5.35\cdot 10^5$ m/s in very good agreement with the calculus of Brinkman et al [10]. In Fig. 7 is shown the fit (solid line) of experimental values, from ref. 26, of H_{c2} at $T = 10$ K. The fit isn't so good because, may be, the approximation of the free electron gas is too strong.

Finally I conclude by summarizing the main points of this paper. I have fitted the experimental critical temperatures as a function of pressure in the framework of two bands Eliashberg theory with only a free parameter. The result is very good. After I have calculated other physical quantities can will be compared with future measurement (for example superconductive gaps from tunneling curves) and I can affirm that the MgB_2 under pressure is, as the same materials in ambient pressure, a moderate coupling two-band phononic systems well described by two-bands Eliashberg theory.

Many thanks are due to A. Calzolari for useful discussions.

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